THEOCHEM, VOLUME 36 (1987)

(Journal of Molecular Structure, Vol. 151)

AUTHOR INDEX

Ando, I. 191

Bala, S. S. 113
Barone, V. 365
Beauchamp, P. S. 297
Bhanuprakash, K. 149
Bock, C. W. 15
Boggs, J. E. 341
Bouchoux, G. 107
Brunvoll, J. 271

Chandra, A. K. 149
Chau, F. T. 157, 173
Cornelisse, J. 1
Coulombeau, C. 331
Cousse, H. 379
Crasnier, F. 379
Császár, A. G. 29
Császár, P. 29
Cyvin, B. N. 271
Cyvin, S. J. 271

Dähne, S. 61
Dinya, Z. 29

Engelmann, A. R. 81

Fabian, J. 355
Faucher, H. 331
Flament, J. P. 39
Fogarasi, G. 341

Gervais, H. P. 39
Ghosh, P. N. 113, 125
Goldstein, E. 297
Graovac, A. 61

Harcourt, R. D. 203
Hase, Y. 223

Jeevan Kumar, R. 103
Junqian, L. 19

Kallel, A. 297
Kovačević, K. 233

Labarre, J.-F. 379
Lahana, R. 379
Leroy, G. 307, 325
Levine, R. D. 385
Liescheski, P. P. 341

Maksić, Z. B. 233
Malatesta, V. 287
Marriott, S. 15
Medina Llanos, C. 81
Mehlhorn, A. 355
Millefiori, A. 373
Millefiori, S. 373
Mitra, K. 125
Mulder, J. J. C. 1
Murthy, V. R. 103

Norinder, U. 259
Nyholm, P. G. 81

Panja, P. K. 113
Párkányi, C. 245
Pascher, I. 81
Patoiseau, J.-F. 379
Peeters, D. 325
Pitet, G. 379
Polansky, O. E. 61
Pulay, P. 341

Raghavan, K. 385
Ranghino, G. 287
Rerat, M. 39
Russo, N. 365

Sacchi, N. 287
Sana, M. 307, 325
Sathyamurthy, N. 385
Silvestro, T. 15
Singh, O. P. 227
Skancke, P. N. 11
Skrezenek, F. L. 203
Somogyi, Á. 29
So, S. P. 141
Subra, R. 365
Szalay, P. G. 341

Tapia, O. 81
Topsom, R. D. 15
Toscano, M. 365
Tosi, C. 287
Tylli, H. 71
Tyutyulkov, N. 355

Van der Hart, J. A. 1
Von Szentpály, L. 245
Vučković, D. Lj. 233
Vujisić, Lj. 233

Williams, G. R. J. 215
Wendan, C. 19
Webb, G. A. 191

Yadav, J. S. 227
Yadav, L. S. 227
Yadav, P. N. S. 227
Yamanobe, T. 191
Younang, E. 325

THEOCHEM VOLUME 36 (1987)

(Journal of Molecular Structure, Vol. 151)

SUBJECT INDEX

Adenine,
a theoretical reinvestigation of the nucleic bases adenine, guanine, cytosine, thymine and uracil using AM1 259
Ammonia—boryl radical,
the structure of the ammonia—boryl radical (BH_2NH_3), an inorganic analogue of the ethyl radical. A non empirical study 365
Antitumour anthracyclines,
redox properties of antitumour anthracyclines as predicted from ab initio calculations and electrochemical experiments 287

Basketanes,
geometry of molecules. Part 8. Interatomic distances, bond angles and hybridization in some basketanes by the IMO method 233
Benzene,
the *meta* photocycloaddition of benzene to ethylene semi-empirical calculations 1
Benzenoid hydrocarbons,
trigonal benzenoid hydrocarbons 271
Bicyclo[3.3.1]nonane,
an ab initio study of bicyclo[3.3.1]-nonane 11

(+)-Car-3-ene,
a conformational study of (+)-car-3-ene: fully optimized STO-3G structures 71
Chlorobenzenes,
bond orders, valence indices and oxidation numbers of some isomeric chlorobenzenes 227
$[C_3H_4O]^{+\cdot}$,
gaseous $[C_3H_4O]^{+\cdot}$ radical cations: expected structures 107
Cholesterol—water interface,
studies on membrane hydration. Part I. Monte Carlo simulation of the cholesterol—water interface 81
CO,
gauge-dependent ket calculations of the magnetic properties of molecules. Part I. Method and application of H_2, H_2O and CO 39
Cyclopentadienyl cations,
the molecular structure of substituted cyclopentadienyl cations 355
Cytosine,
a theoretical reinvestigation of the nucleic bases adenine, guanine, cytosine, thymine and uracil using AM1 259

2,5-Dimercapto-1,3,4-thiadiazole,
an ab initio study of the tautomeric equilibria and structure of 2,5-dimercapto-1,3,4-thiadiazole 373
Dizatrifone,
theoretical conformational analysis and antalgic activity of a new triazinic derivative dizatrifone and related compounds 379

Ethylene dimer- and trimer-cations,
an ab initio study with counterpoise correction of ethylene dimer- and trimer-cations 149
Ethylene,
The *meta* photocycloaddition of benzene to ethylene semi-empirical calculations 1

Fermi resonance studies,
temperature-dependent Fermi resonance studies and lineshape simulation by random perturbation model 113
2-Fluorovinyl radicals,
calculation of one vibrational frequency of the *cis* and *trans* 2-fluorovinyl radicals 331

Guanine,
a theoretical reinvestigation of the nucleic bases adenine, guanine, cytosine, thymine and uracil using AM1 259

HCN—BF_3,
theoretical study of the coordination effect: the C≡N bond stretch force

constants of HCN—BF_3 and HCN—BCl_3 223

N-Heteroaromatic polycycles,
the MCS model of chemical initiation of cancer: PPP calculations on methylated and *N*-heteroaromatic polycycles 245

Hexatriene,
scaled quantum mechanical (SQM) force field and vibrational assignment for hexatriene 341

H_2,
gauge-dependent ket calculations of the magnetic properties of molecules. Part I. Method and application of H_2, H_2O and CO 39

H_2O,
gauge-dependent ket calculations of magnetic properties of molecules. Part I. Method and Application of H_2, H_2O and CO 39

Hydrogen oxide,
validity of Franck—Condon analysis procedures for deduction of excited-state and ionic geometries. Part II. The X^2B_1 and A^2A_1 states of hydrogen oxide and hydrogen sulphur 173

Hydrogen sulphur,
validity of Franck—Condon analysis procedures for deduction of excited-state and ionic geometries. Part II. The X^2B_1 and A^2A_1 states of hydrogen oxide and hydrogen sulphur 173

Li,
nonlinear surprisal for product vibrational state distribution for the reaction Li + FH → LiF + H 385

Monosubstituted benzenes,
calculated dipole moments for monosubstituted benzenes 15

Monothioformic acids,
structures, relative stabilities and barriers to internal rotation of isomeric monothioformic acids 141

N_2O,
validity of Franck—Condon analysis procedures for deduction of excited-state and ionic geometries I. The $X^2\Pi$ and $A^2\Sigma^+$ states of N_2O 157

Organic π-electron systems,
finite field calculations of molecular polarizability and hyperpolarizabilities for organic π-electron systems 215

Planar frame molecules,
molecular symmetry group, selection rules and vibration—rotation band envelopes of molecules with planar frame and C_{3v} type free internal rotation 125

Polyacetylenes,
^{13}C NMR chemical shifts and electronic structure of *cis* and *trans* polyacetylenes as studied by tight-binding within the INDO/s framework 191

Polymethines,
topological effect on MO energies. Part 14. Topological MO-effect in intramolecularly coupled polymethines 61

4H-Pyran-4-one,
theoretical force fields and vibrational spectra of 4H-pyran-4-one by CNDO/2 and MINDO/3 force methods 29

α-Pyrone,
theoretical study of the mechanism of the cycloaddition of acetylene to α-pyrone asynchronism and substituent effects 297

Small molecules and ions,
a theoretical investigation of the nuclear and electronic structure of some $XYH_n^{(a)}$ small molecules and ions 307

Small molecules and radicals,
heats of formation of some small molecules and radicals 325

S_2N_2,
S_2N_2 and S_4^{2+}: some further valence bond studies 203

Substituted benzenes,
magneto-optic rotatory dispersion — studies of some substituted benzenes by a new dispersion relation 103

Thymine,
a theoretical reinvestigation of the nucleic bases adenine, guanine, cytosine, thymine and uracil using AM1 259

Transition metal cluster,
a study of bonding effect between the metal—metal in the transition metal cluster 19

Uracil,
a theoretical reinvestigation of the nucleic bases adenine, guanine, cytosine, thymine and uracil using AM1 259

CONTENTS

The *meta* photocycloaddition of benzene to ethylene semi-empirical calculations
J. A. van der Hart, J. J. C. Mulder and J. Cornelisse (Leiden, The Netherlands) 1

An ab initio study of bicyclo[3.3.1]nonane
P. N. Skancke (Tromsø, Norway) 11

Calculated dipole moments for monosubstituted benzenes
S. Marriott, T. Silvestro, R. D. Topsom (Bundoora, Australia) and C. W. Bock (Philadelphia, PA, U.S.A.) . . . 15

A study of bonding effect between the metal—metal in the transition metal cluster
L. Junqian and C. Wendan (Fujian, China) 19

Theoretical force fields and vibrational spectra of 4H-pyran-4-one by CNDO/2 and MINDO/3 force methods
Á. Somogyi, Z. Dinya (Debrecen, Hungary), P. Császár (St. John's Canada) and A. G. Császár (Corvallis, OR, U.S.A.) 29

Gauge-dependent ket calculation of the magnetic properties of molecules. Part I. Method and application to H_2, H_2O and CO
J. P. Flament, H. P. Gervais and M. Rerat (Palaiseau, France) 39

Topological effect on MO energies. Part 14. Topological MO-effect in intramolecularly coupled polymethines
S. Dähne (Berlin, G.D.R.), A. Graovac and O. E. Polansky (Ruhr, F.R.G.) 61

A conformational study of (+)-car-3-ene: fully optimized STO-3G structures
H. Tylli (Helsinki, Finland) 71

Studies on membrane hydration. Part I. Monte Carlo simulation of the cholesterol—water interface
A. R. Engelmann, C. Medina Llanos, O. Tapia (Uppsala, Sweden), P. G. Nyholm and I. Pascher (Gothenburg, Sweden) 81

Magneto-optic rotatory dispersion — studies of some substituted benzenes by a new dispersion relation
V. R. Murthy and R. Jeevan Kumar (Anantapur, India) 103

Gaseous $[C_3H_4O]^{+\cdot}$ radical cations: expected structures
G. Bouchoux (Palaiseau, France) 107

Temperature-dependent Fermi resonance studies and lineshape simulation by random perturbation model
S. S. Bala, P. K. Panja and P. N. Ghosh (Calcutta, India) 113

Molecular symmetry group, selection rules and vibration—rotation band envelopes of molecules with planar frame and C_{3v} type free internal rotation
K. Mitra and P. N. Ghosh (Calcutta, India) 125

Structures, relative stabilities and barriers to internal rotation of isomeric monothioformic acids
S. P. So (Shatin, Hong Kong) 141

An ab initio study with counterpoise correction of ethylene dimer- and trimer-cations
A. K. Chandra and K. Bhanuprakash (Bangalore, India) 149

Validity of Franck—Condon analysis procedures for deduction of excited-state and ionic geometries I. The $X^2\Pi$ and $A^2\Sigma^+$ states of N_2O
F. T. Chau (Hung Hom, Hong Kong) 157

Validity of Franck—Condon analysis procedures for deduction of excited-state and ionic geometries. Part II. The X^2B_1 and A^2A_1 states of hydrogen oxide and hydrogen sulphur
F. T. Chau (Hung Hom, Hong Kong) 173

^{13}C NMR chemical shifts and electronic structure of *cis* and *trans* polyacetylenes as studied by tight-binding theory within the INDO/s framework
T. Yamanobe, I. Ando (Tokyo, Japan) and G. A. Webb (Guildford, Gt. Britain) 191

S_2N_2 and S_4^{2+}: some further valence bond studies
R. D. Harcourt and F. L. Skrezenek (Parkville, Vic., Australia) 203

Finite field calculations of molecular polarizability and hyperpolarizabilities for organic π-electron systems
G. R. J. Williams (Adelaide, S.A., Australia) 215

Theoretical study of the coordination effect: the C≡N bond stretch force constants of HCN–BF_3 and HCN–BCl_3
Y. Hase (Campinas, Brazil) 223
Bond orders, valence indices and oxidation numbers of some isomeric chlorobenzenes
L. S. Yadav, O. P. Singh, P. N. S. Yadav (Varanasi, India) and J. S. Yadav (Newark, NJ, U.S.A.) 227
Geometry of molecules. Part 8. Interatomic distances, bond angles and hybridization in some basketanes by the IMO method
K. Kovačević and Z. B. Maksić (Zagreb, Yugoslavia), D. Lj. Vučković and Lj. Vujisić (Beograd, Yugoslavia) . . 233
The MCS model of chemical initiation of cancer: PPP calculations on methylated and *N*-heteroaromatic polycycles
L. von Szentpály and C. Párkányi (El Paso, TX, U.S.A.) 245
A theoretical reinvestigation of the nucleic bases adenine, guanine, cytosine, thymine and uracil using AM1
U. Norinder (Södertälje, Sweden) 259
Trigonal benzenoid hydrocarbons
S. J. Cyvin, B. N. Cyvin and J. Brunvoll (Trondheim, Norway) 271
Redox properties of antitumour anthracyclines as predicted from ab initio calculations and electrochemical experiments
G. Ranghino, C. Tosi (Novara, Italy), V. Malatesta and N. Sacchi (Milano, Italy) 287
Theoretical study of the mechanism of the cycloaddition of acetylene to α-pyrone: asynchronism and substituent effects
E. Goldstein, A. Kallel and P. S. Beauchamp (Pomona, CA, U.S.A.) 297
A theoretical investigation of the nuclear and electronic structure of some $XYH_n^{(q)}$ small molecules and ions
M. Sana and G. Leroy (Louvain-la-Neuve, Belgium) 307
Heats of formation of some small molecules and radicals
M. Sana, G. Leroy, D. Peeters and E. Younang (Louvain-la-Neuve, Belgium) 325
Calcul d'une vibration des radicaux fluoro-2 vinyles *cis* et *trans*
C. Coulombeau and H. Faucher (Saint Martin d'Heres, France) 331
Scaled quantum mechanical (SQM) force field and vibrational assignment for hexatriene
G. Fogarasi, P. G. Szalay (Budapest, Hungary), P. P. Liescheski, J. E. Boggs (Austin, TX, U.S.A.) and P. Pulay (Fayetteville, AR, U.S.A.) 341
The molecular structure of substituted cyclopentadienyl cations
J. Fabian, A. Mehlhorn (Dresden, G.D.R.) and N. Tyutyulkov (Sofia, Bulgaria) 355
The structure of the ammonia–boryl radical (BH_2NH_3), an inorganic analogue of the ethyl radical. A non empirical study
N. Russo, R. Subra, M. Toscano (Arcavacata di Rende, Italy) and V. Barone (Napoli, Italy) 365

Short communications

An ab initio study of the tautomeric equilibria and structure of 2,5-dimercapto-1,3,4-thiadiazole
S. Millefiori and A. Millefiori (Catania, Italy) 373
Theoretical conformational analysis and antalgic activity of a new triazinic derivative dizatrifone and related compounds
R. Lahana, F. Crasnier, J.-F. Labarre (Toulouse, France), H. Cousse, G. Pitet and J.-F. Patoiseau (Castres, France) 379
Nonlinear surprisal for product vibrational state distribution for the reaction Li + FH → LiF + H
K. Raghavan, N. Sathyamurthy (Kanpur, India) and R. D. Levine (Jerusalem, Israel) 385

Book reviews 391

Author index 395

Subject index 396